

Structure search in REGISTRY (^{Cross to CAPlus USPatFull})

Berch 10_716141

12/15/2005

=> file registry

FILE 'REGISTRY' ENTERED AT 16:43:20 ON 15 DEC 2005
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STRUCTURE FILE UPDATES: 14 DEC 2005 HIGHEST RN 869939-98-0
DICTIONARY FILE UPDATES: 14 DEC 2005 HIGHEST RN 869939-98-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

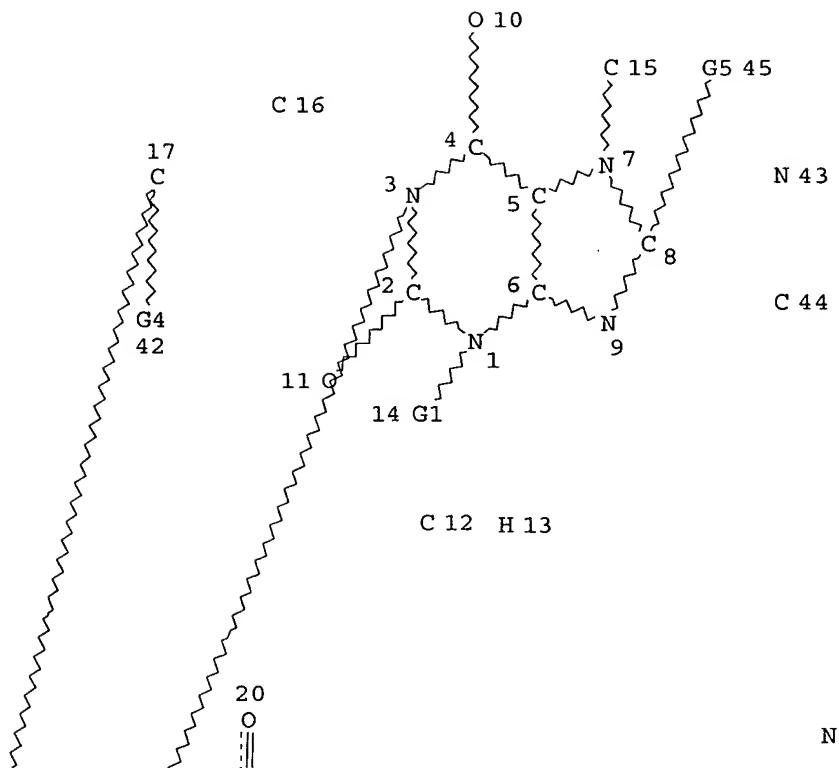
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

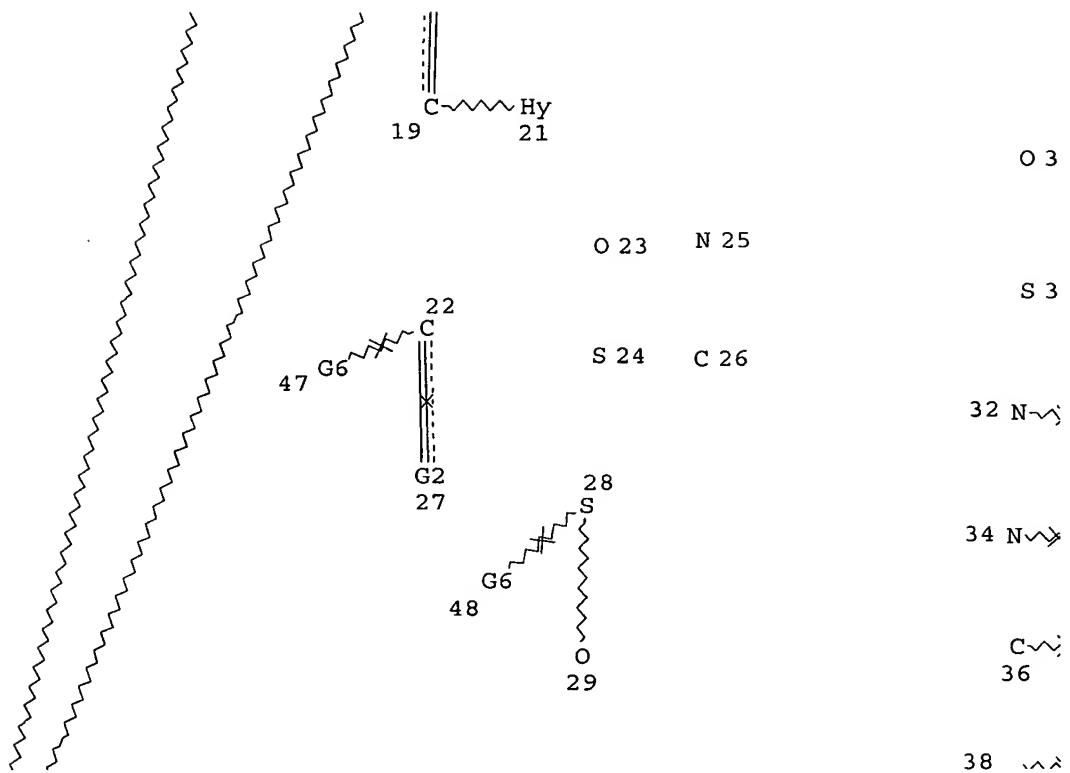
=> d stat que L29
L12 STR



Page 1-A

6

Page 1-B



Page 2-A
30

31

~X~N 33

~X~O 35

~X~O
37

~A~

Page 2-B

18 G20

38 C~;

40 C~;

Page 3-A

~X~S 39

~X~N 41

Page 3-B
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VAR G2=23/24/25/26
VAR G4=19/22/28
VAR G5=43/44
VAR G6=30/31/32/34/36/38/40/46
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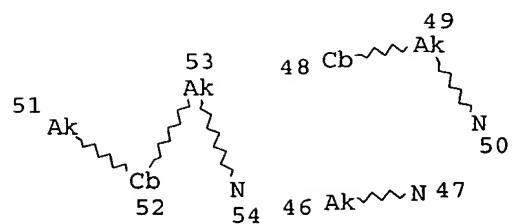
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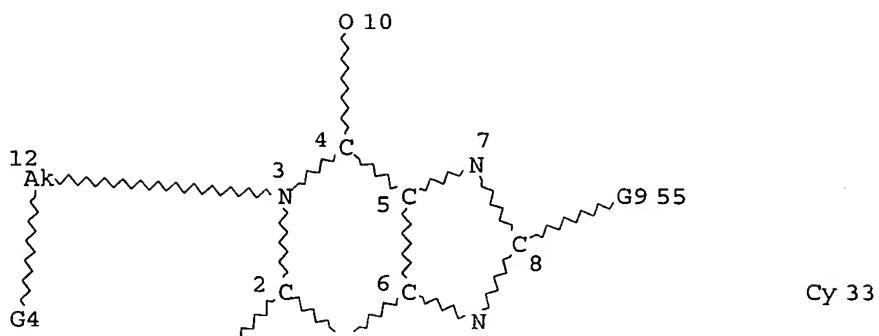
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NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

L14 866 SEA FILE=REGISTRY SSS FUL L12
L27 STR



N 45



Page 1-A



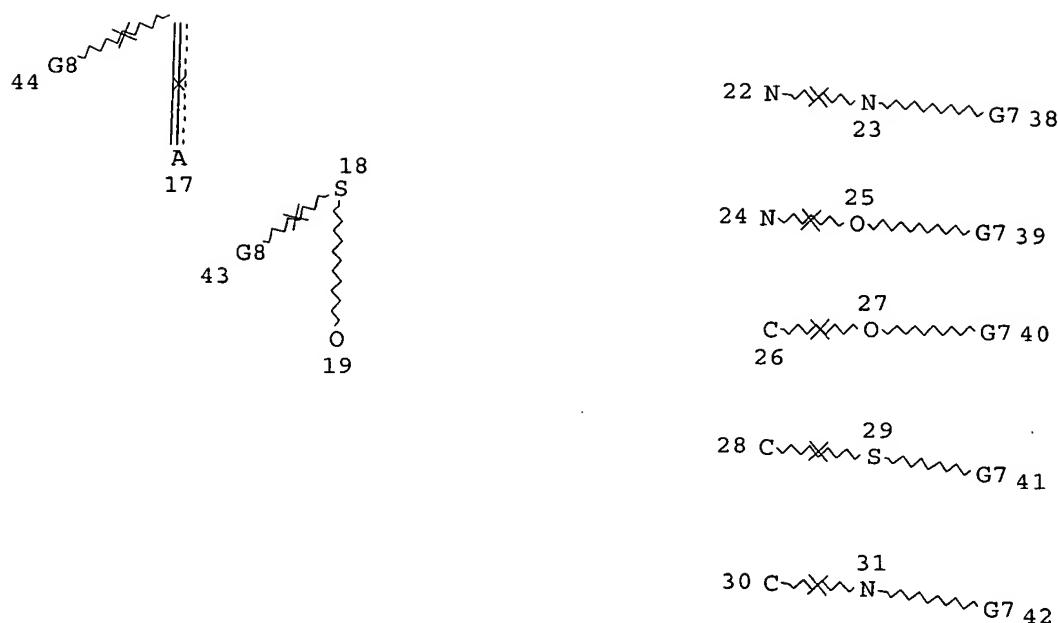
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21 S~~~~~ G7 37

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Page 2-A



Page 3-A

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VAR G9=45/46/48/51

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DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1 N  AT  15

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GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 55

STEREO ATTRIBUTES: NONE

L29 29 SEA FILE=REGISTRY SUB=L14 SSS FUL L27

100.0% PROCESSED 866 ITERATIONS
 SEARCH TIME: 00.00.01

29 ANSWERS

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TERM #  # OCC  # DOC  % DOC LC
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2      27      27  93.10 CAPLUS
3      17      17  58.62 USPATFULL
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FILE LAST UPDATED: 14 Dec 2005 (20051214/ED)

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<http://www.cas.org/infopolicy.html>
'OBJ' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

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L14      866 SEA FILE=REGISTRY SSS FUL L12
L27      STR
L29      29 SEA FILE=REGISTRY SUB=L14 SSS FUL L27
L30      4 SEA FILE=CAPLUS ABB=ON PLU=ON L29
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=> file uspatfull
FILE 'USPATFULL' ENTERED AT 16:43:50 ON 15 DEC 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 15 Dec 2005 (20051215/PD)
FILE LAST UPDATED: 15 Dec 2005 (20051215/ED)
HIGHEST GRANTED PATENT NUMBER: US6976271
HIGHEST APPLICATION PUBLICATION NUMBER: US2005278816
CA INDEXING IS CURRENT THROUGH 15 Dec 2005 (20051215/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 15 Dec 2005 (20051215/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2005

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>>> USPAT2 is now available. USPATFULL contains full text of the      <<<
>>> original, i.e., the earliest published granted patents or      <<<
>>> applications. USPAT2 contains full text of the latest US      <<<
>>> publications, starting in 2001, for the inventions covered in      <<<
>>> USPATFULL. A USPATFULL record contains not only the original      <<<
>>> published document but also a list of any subsequent      <<<
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>>> publications. The publication number, patent kind code, and <<<
 >>> publication date for all the US publications for an invention <<<
 >>> are displayed in the PI (Patent Information) field of USPATFULL <<<
 >>> records and may be searched in standard search fields, e.g., /PN, <<<
 >>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<
 >>> through the new cluster USPATALL. Type FILE USPATALL to <<<
 >>> enter this cluster. <<<

>>> <<<
 >>> Use USPATALL when searching terms such as patent assignees, <<<
 >>> classifications, or claims, that may potentially change from <<<
 >>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> d que nos L35
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L27      STR
L29      29 SEA FILE=REGISTRY SUB=L14 SSS FUL L27
L35      3 SEA FILE=USPATFULL ABB=ON PLU=ON L29
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FILE 'CAPLUS' ENTERED AT 16:44:10 ON 15 DEC 2005
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FILE 'USPATFULL' ENTERED AT 16:44:10 ON 15 DEC 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
PROCESSING COMPLETED FOR L30
PROCESSING COMPLETED FOR L35
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          ANSWERS '5-7' FROM FILE USPATFULL
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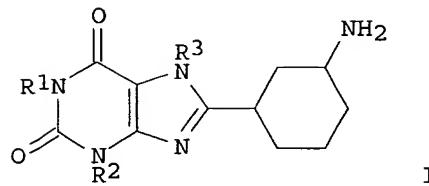
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L36 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:182879 CAPLUS
DOCUMENT NUMBER: 140:235743
TITLE: Preparation of 8-[3-aminopiperidin-1-yl]xanthines as
       dipeptidylpeptidase-IV (DPP-IV) inhibitors.
INVENTOR(S): Himmelsbach, Frank; Langkopf, Elke; Eckhardt,
              Matthias; Mark, Michael; Maier, Roland; Lotz, Ralf
              Richard Hermann; Tadayyon, Mohammad
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G.,
                     Germany
SOURCE: PCT Int. Appl., 226 pp.
        CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:
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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004018468	A2	20040304	WO 2003-EP9127	20030818
WO 2004018468	A3	20040408		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10238243	A1	20040304	DE 2002-10238243	20020821
DE 10312353	A1	20040930	DE 2003-10312353	20030320
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EP 1532149	A2	20050525	EP 2003-792359	20030818
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NO 2005000069	A	20050303	NO 2005-69	20050106
PRIORITY APPLN. INFO.:				
			DE 2002-10238243	A 20020821
			DE 2003-10312353	A 20030320
			WO 2003-EP9127	W 20030818

OTHER SOURCE(S) : MARPAT 140:235743
GI



AB Title compds. (I; R1 = Me substituted by Me2NCO, pyrrolidin-1-ylcarbonyl, piperidin-1-ylcarbonyl, tert-butyloxycarbonyl, naphthyl, nitronaphthyl, dimethylaminonaphthyl, phenoxydiazolyl, quinolinyl, indolyl, cinnolinyl, benzothienyl, etc.; R2 = Me, Me2CH, Ph; R3 = 2-methyl-2-propenyl, 2-chloro-2-propenyl, 3-bromo-2-propenyl, 2-butenyl, 2,3-dimethyl-2-butenyl, 2-butynyl, 1-cyclopentenylmethyl, 2-furylmethyl), were prepared. Thus, 1,3-dimethyl-7-(2,6-dicyanobenzyl)-8-bromoxanthine (preparation from 8-bromotheophylline and 2-bromomethylisophthalonitrile given), 3-aminopiperidine dihydrochloride, and K2CO3 were heated in DMF for 3 h at 80° to give 14% 1,3-dimethyl-7-(2,6-dicyanobenzyl)-8-(3-aminopiperidin-1-yl)xanthine. I inhibited DPP-IV with IC50 = 1-2160 nM.

IT 668270-29-9P 668270-98-2P 668271-03-2P
668271-15-6P 668271-65-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

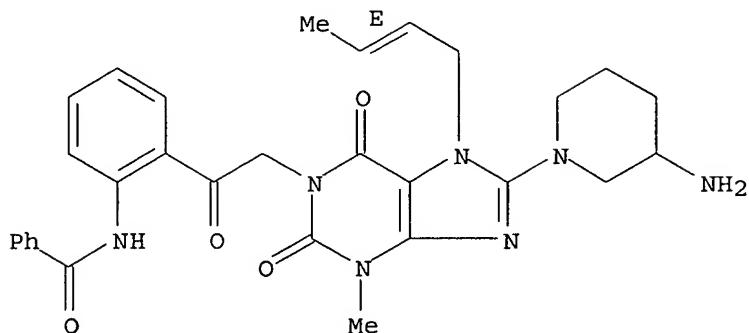
(preparation of aminopiperidinylxanthines as dipeptidylpeptidase-IV inhibitors)

RN 668270-29-9 CAPLUS

CN Benzamide, N-[2-[(8-(3-amino-1-piperidinyl)-7-(2E)-2-butenoxy-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl)acetyl]phenyl]- (9CI) (CA

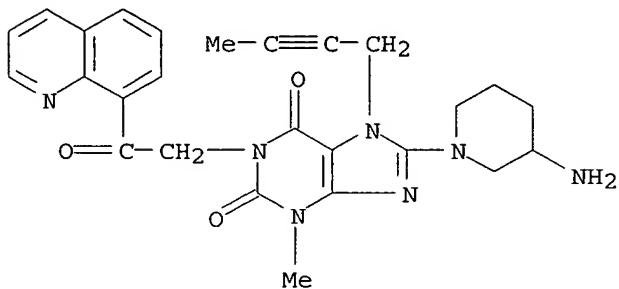
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Double bond geometry as shown.



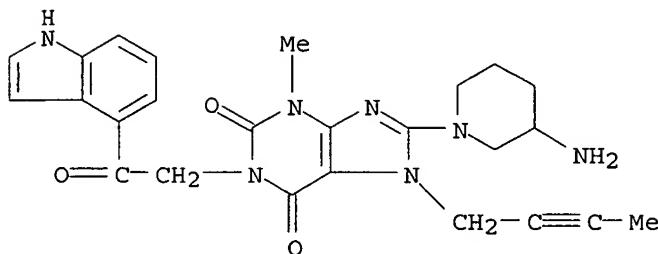
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CN 1H-Purine-2,6-dione, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-3,7-dihydro-3-methyl-1-[2-oxo-2-(8-quinolinyl)ethyl]- (9CI) (CA INDEX NAME)



RN 668271-03-2 CAPLUS

CN 1H-Purine-2,6-dione, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-3,7-dihydro-1-[2-(1H-indol-4-yl)-2-oxoethyl]-3-methyl- (9CI) (CA INDEX NAME)



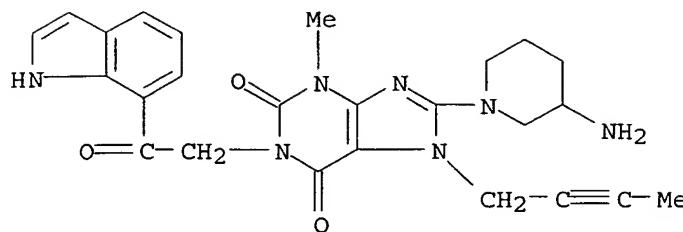
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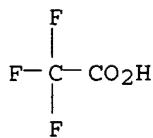
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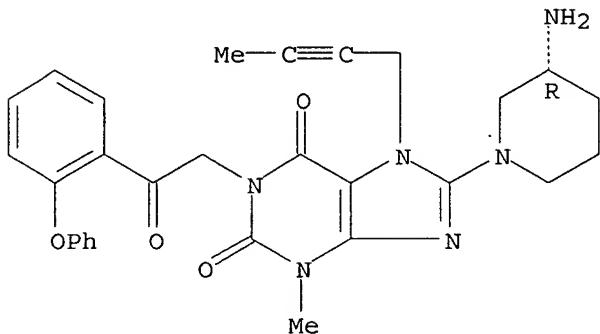


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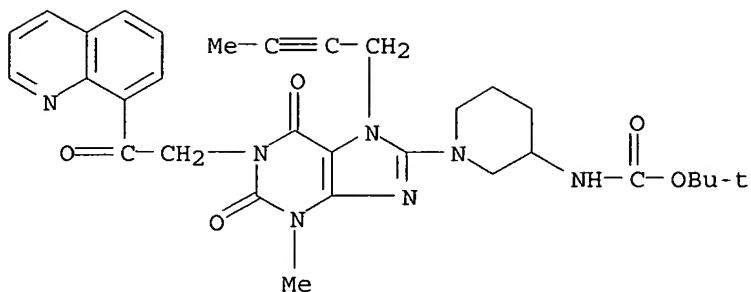
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RN 668271-65-6 CAPLUS
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Absolute stereochemistry.

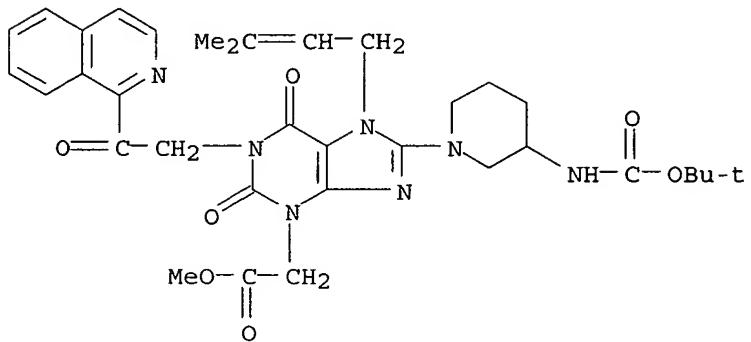


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 (preparation of aminopiperidinylxanthines as dipeptidylpeptidase-IV inhibitors)
 RN 668272-79-5 CAPLUS
 CN Carbamic acid, [1-[7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-[2-oxo-2-(8-quinolinyl)ethyl]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



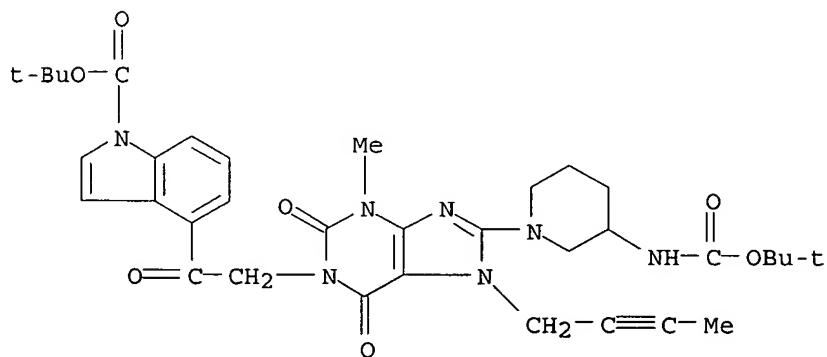
RN 668273-56-1 CAPLUS

CN 3H-Purine-3-acetic acid, 8-[3-[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl-1,2,6,7-tetrahydro-1-[2-(1-isoquinolinyl)-2-oxoethyl]-7-(3-methyl-2-butynyl)-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 668274-25-7 CAPLUS

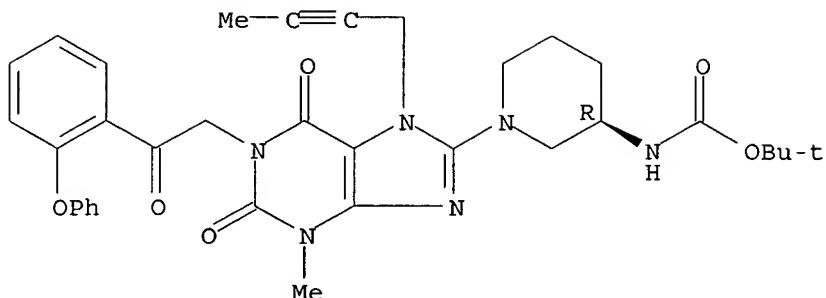
CN 1H-Indole-1-carboxylic acid, 4-[[7-(2-butynyl)-8-[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 668274-76-8 CAPLUS

CN Carbamic acid, [(3R)-1-[7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-[2-oxo-2-(2-phenoxyphenyl)ethyl]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

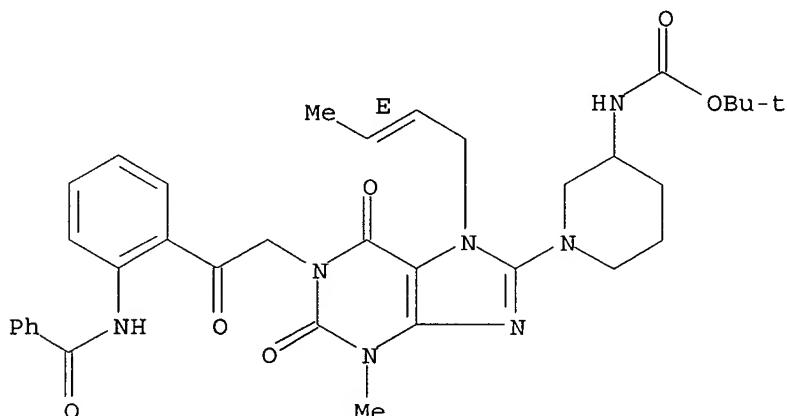
Absolute stereochemistry.



RN 668275-19-2 CAPLUS

CN Carbamic acid, [1-[1-[2-[2-(benzoylamino)phenyl]-2-oxoethyl]-7-(2E)-2-butenyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L36 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:450501 CAPLUS

DOCUMENT NUMBER: 141:23542

TITLE: Preparation of xanthine derivatives as dipeptidylpeptidase IV inhibitors

INVENTOR(S): Eckhardt, Matthias; Himmelsbach, Frank; Langkopf, Elke; Maier, Roland; Mark, Michael; Tadayyon, Mohammad

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. Kg, Germany

SOURCE: Ger. Offen., 31 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

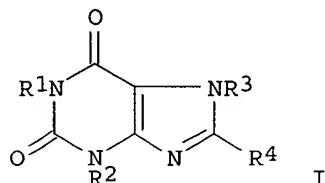
This work

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10254304	A1	20040603	DE 2002-10254304	20021121

WO 2004046148	A1	20040603	WO 2003-EP12821	20031111
WO 2004046148	C1	20050714		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1565468	A1	20050824	EP 2003-782204	20031111
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CA 2506720	AA	20040603	CA 2003-2506720	20031117
US 2004138215	A1	20040715	US 2003-716141	20031118
PRIORITY APPLN. INFO.:			DE 2002-10254304	A 20021121
			US 2002-432450P	P 20021211
			WO 2003-EP12821	W 20031111

OTHER SOURCE(S) : MARPAT 141:23542

GI



AB Title compds. [I; R1 = ABD; A = (substituted) alkyl, etc.; B = EG; E = O, S, etc.; G = (thio)carbonyl, (imino-substituted) Me, etc.; D = propionyl, (fluorinated) alkyl, alkenyl; R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, etc.; R3 = (substituted) alkyl, aryl, furanyl, thieryl, oxazolyl, isoxazolyl, etc.; R4 = (substituted) azetidin-1-yl, pyrrolidin-1-yl, piperidin-1-yl, etc.], were prepared. Thus, 1-[(benzyloxycarbonyl)methyl]-3-methyl-7-(2-butyn-1-yl)-8[(R)-3-(tert-butyloxycarbonylamino)piperidin-1-yl]xanthine (preparation given) in CH₂Cl₂ was shaken with CF₃CO₂H for 20 min at 30° to give 97% 1-[(benzyloxycarbonyl)methyl]-3-methyl-7-(2-butyn-1-yl)-8[(R)-3-aminopiperidin-1-yl]xanthine. The latter inhibited dipeptidylpeptidase IV (DPP IV) with IC₅₀ = 27 nM.

IT 697806-80-7P 697806-84-1P 697806-90-9P
 697806-92-1P 697806-93-2P 697806-95-4P
 697806-96-5P

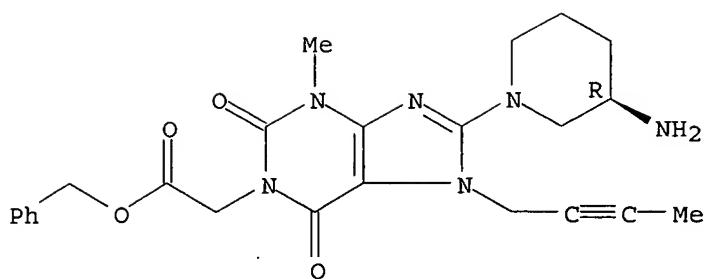
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of xanthine derivs. as dipeptidylpeptidase IV inhibitors)

RN 697806-80-7 CAPLUS

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

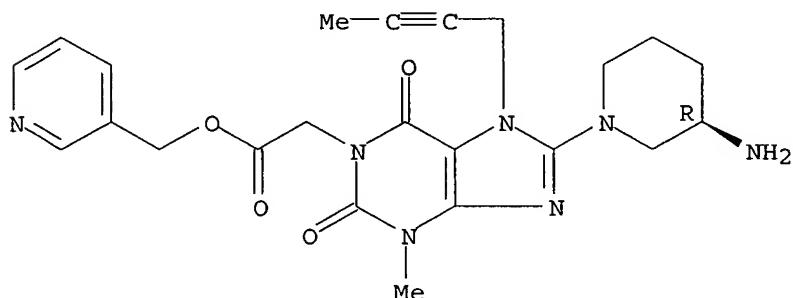
Absolute stereochemistry.



RN 697806-84-1 CAPLUS

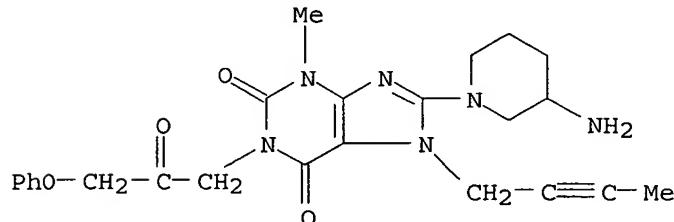
CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, 3-pyridinylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 697806-90-9 CAPLUS

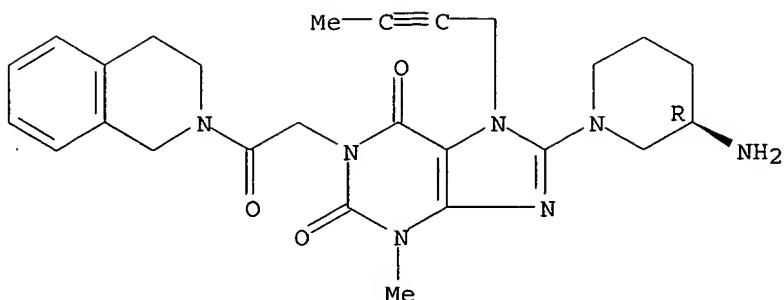
CN 1H-Purine-2,6-dione, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-3,7-dihydro-3-methyl-1-(2-oxo-3-phenoxypropyl)- (9CI) (CA INDEX NAME)



RN 697806-92-1 CAPLUS

CN Isoquinoline, 2-[[8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

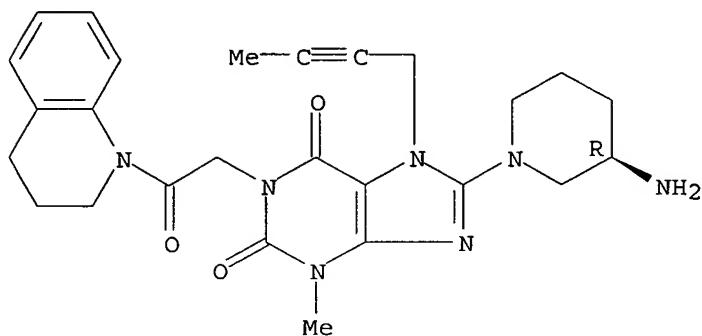
Absolute stereochemistry.



RN 697806-93-2 CAPLUS

CN Quinoline, 1-[(8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

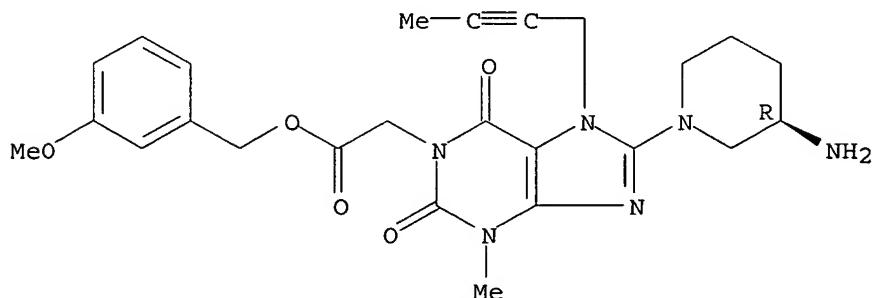
Absolute stereochemistry.



RN 697806-95-4 CAPLUS

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

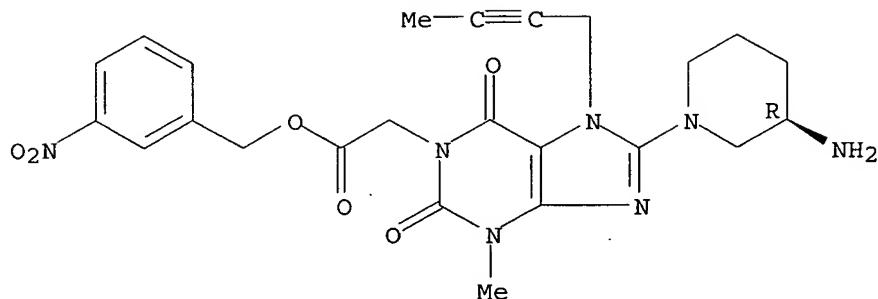
Absolute stereochemistry.



RN 697806-96-5 CAPLUS

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 697806-55-6P 697806-59-0P 697806-67-0P
 697806-68-1P 697806-72-7P 697806-75-0P
 697806-76-1P

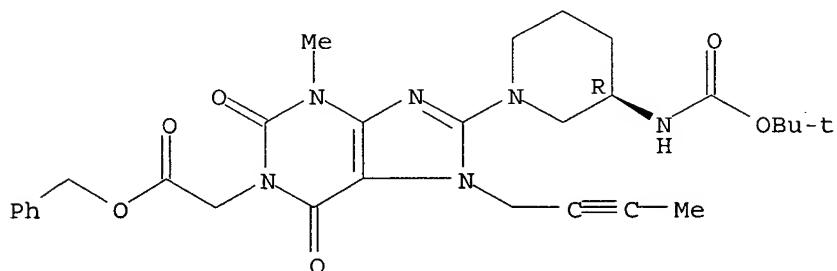
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of xanthine derivs. as dipeptidylpeptidase IV inhibitors)

RN 697806-55-6 CAPLUS

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

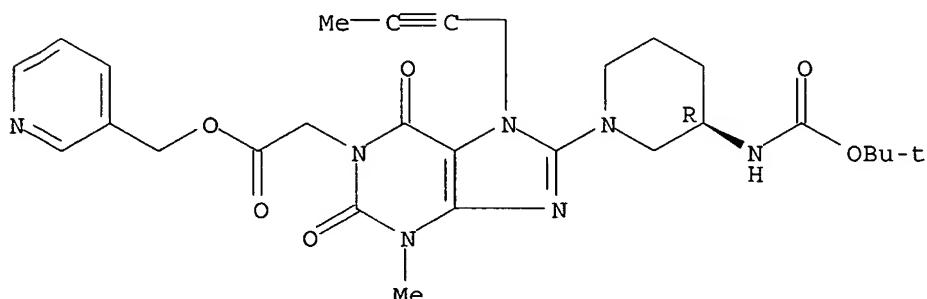
Absolute stereochemistry.



RN 697806-59-0 CAPLUS

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, 3-pyridinylmethyl ester (9CI) (CA INDEX NAME)

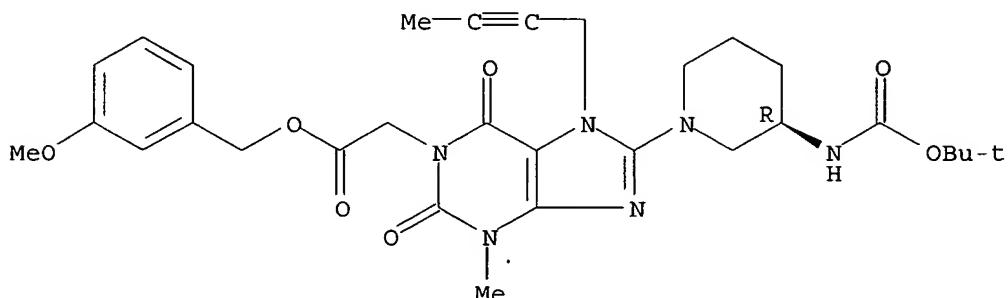
Absolute stereochemistry.



RN 697806-67-0 CAPLUS

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

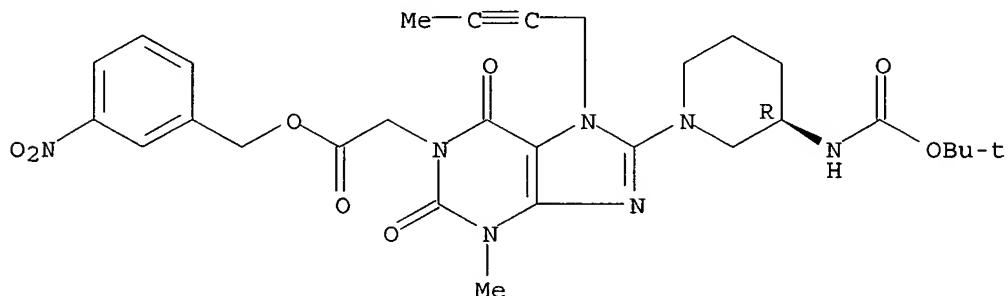
Absolute stereochemistry.



RN 697806-68-1 CAPLUS

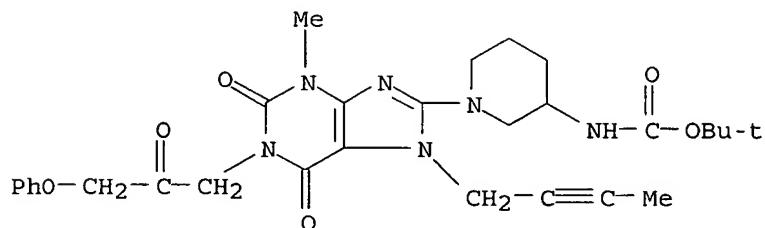
CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 697806-72-7 CAPLUS

CN Carbamic acid, [1-[7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-3-phenoxypropyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

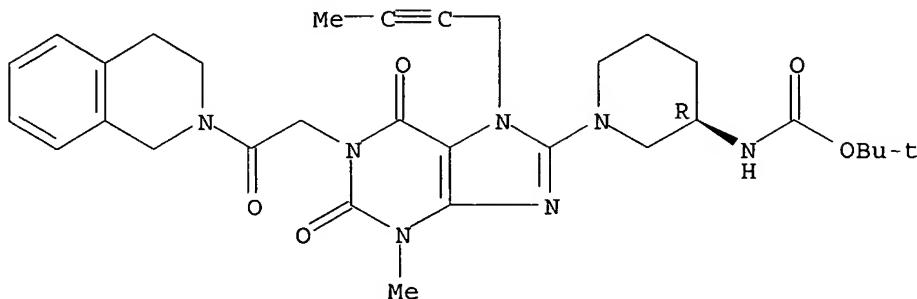


RN 697806-75-0 CAPLUS

CN Carbamic acid, [(3R)-1-[7-(2-butynyl)-1-[2-(3,4-dihydro-2(1H)-isoquinolinyl)-2-oxoethyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-

8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

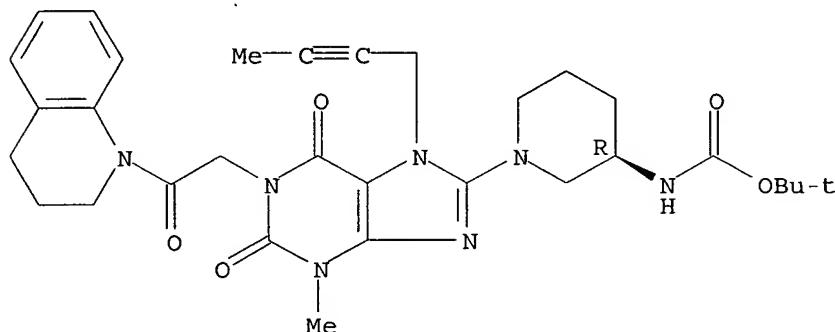
Absolute stereochemistry.



RN 697806-76-1 CAPLUS

CN Carbamic acid, [(3R)-1-[7-(2-butynyl)-1-[2-(3,4-dihydro-1(2H)-quinoliny)-2-oxoethyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L36 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:177908 CAPLUS

DOCUMENT NUMBER: 140:235733

TITLE: Preparation of xanthines as dipeptidylpeptidase IV inhibitors for the treatment of diabetes

INVENTOR(S): Eckhardt, Matthias; Himmelsbach, Frank; Langkopf, Elke; Maier, Roland; Mark, Michael; Lotz, Ralf

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G., Germany

SOURCE: Ger. Offen., 22 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

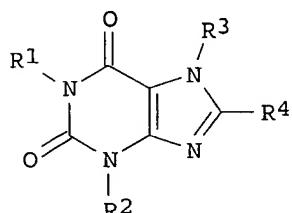
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10238470	A1	20040304	DE 2002-10238470	20020822
US 2004166125	A1	20040826	US 2003-636088	20030807

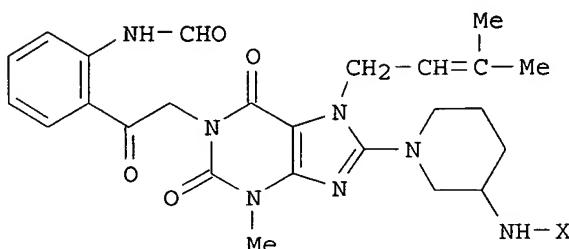
CA 2496325	AA 20040304	CA 2003-2496325	20030816
WO 2004018467	A2 20040304	WO 2003-EP9096	20030816
WO 2004018467	A3 20040513		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1554278	A2 20050720	EP 2003-792342	20030816
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
PRIORITY APPLN. INFO.:		DE 2002-10238470	A 20020822
		US 2002-409258P	P 20020909
		WO 2003-EP9096	W 20030816

OTHER SOURCE(S) : MARPAT 140:235733

GI



I



II

AB Title compds. I [R1 = (un)substituted phenylcarbonylmethyl; R2 = H, alkyl, alkenyl, etc.; R3 = (un)substituted alkyl; R4 = (un)substituted azetidin-1-yl, pyrrolidin-1-yl] and their pharmaceutically acceptable salts were prepared. For example, BOC deprotection of amine II (X = Boc), e.g., prepared from 3-Methyl-8-chloroxanthine, via TFA afforded claimed xanthine II (X = H) in 87% yield. In dipeptidylpeptidase IV inhibition assays, 7-examples of compds. I exhibited IC50 values ranging from 3-11 nM, e.g., the IC50 value of xanthine II (X = H) was 5 nM. Compds. I are claimed useful for the treatment of type I and type II diabetes.

IT 666816-82-6P

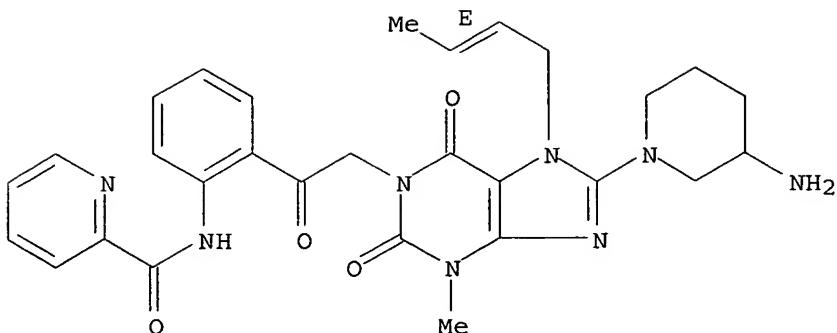
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of xanthines as dipeptidylpeptidase IV inhibitors for the treatment of diabetes)

RN 666816-82-6 CAPLUS

CN 2-Pyridinecarboxamide, N-[2-[[8-(3-amino-1-piperidinyl)-7-(2E)-2-butenyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



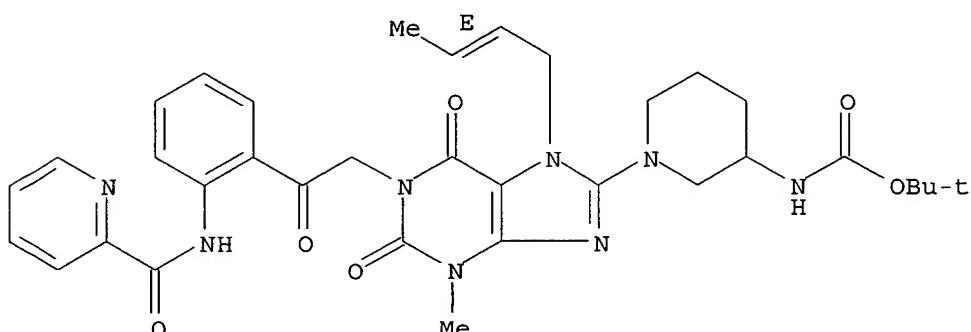
IT 666817-05-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of xanthines as dipeptidylpeptidase IV inhibitors for the treatment of diabetes)

RN 666817-05-6 CAPLUS

CN Carbamic acid, [1-[7-(2E)-2-butenyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-[2-oxo-2-[(2-pyridinylcarbonyl)amino]phenyl]ethyl]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L36 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:675555 CAPLUS

DOCUMENT NUMBER: 139:197299

TITLE: Preparation of xanthine derivatives as DPP-IV inhibitors

INVENTOR(S): Yoshikawa, Seiji; Emori, Eita; Matsuura, Fumiyo; Clark, Richard; Ikuta, Hironori; Yasuda, Nobuyuki; Nagakura, Tadashi; Yamazaki, Kazuto; Aoki, Mika

PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 217 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

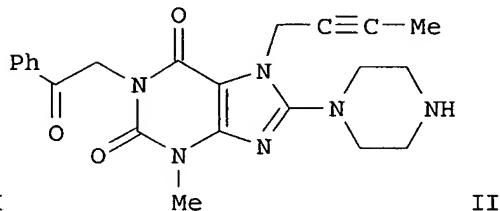
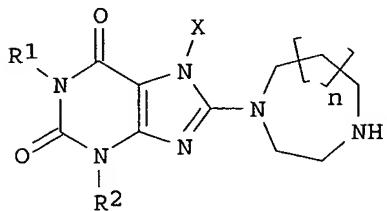
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 1338595	A2	20030827	EP 2003-290431	20030224
EP 1338595	A3	20031008		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004043429	A2	20040212	JP 2003-44771	20030221
US 2004082570	A1	20040429	US 2003-374918	20030224
JP 2002-47761 A 20020225				
JP 2002-149557 A 20020523				

PRIORITY APPLN. INFO.: MARPAT 139:197299

GI



AB Novel xanthine derivs. of formula I [R1, R2 = H, alkyl, alkoxy, hydroxyalkyl, cycloalkyl, aryl, etc.; X = alkynyl, (substituted) Ph; n = 0, 1] are prepared which exhibit an excellent dipeptidyl peptidase IV (DPPIV) inhibition effect. Thus, II was prepared, and inhibited DPPIV with IC50 of 0.654 nM, and improved glucose tolerance in mice by 49.4%.

IT 586402-89-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of xanthine derivs. as DPPIV inhibitors)

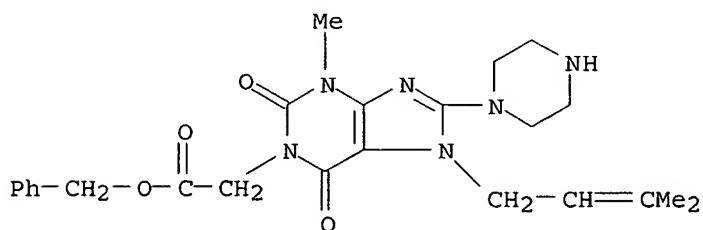
RN 586402-89-3 CAPLUS

CN 1H-Purine-1-acetic acid, 2,3,6,7-tetrahydro-3-methyl-7-(3-methyl-2-butenyl)-2,6-dioxo-8-(1-piperazinyl)-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

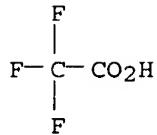
CRN 586402-88-2
CMF C24 H30 N6 O4

*Provided
out*



CM 2

CRN 76-05-1
CMF C2 H F3 O2



L36 ANSWER 5 OF 7 USPATFULL on STN

ACCESSION NUMBER: 2004:215019 USPATFULL
 TITLE: Xanthine derivatives, their preparation and their use
 in pharmaceutical compositions
 INVENTOR(S): Himmelsbach, Frank, Mittelbiberach, GERMANY, FEDERAL
 REPUBLIC OF
 Langkopf, Elke, Warthausen, GERMANY, FEDERAL REPUBLIC
 OF
 Eckhardt, Matthias, Biberach, GERMANY, FEDERAL REPUBLIC
 OF
 Mark, Michael, Biberach, GERMANY, FEDERAL REPUBLIC OF
 Maier, Roland, Biberach an der Riss, GERMANY, FEDERAL
 REPUBLIC OF
 Lotz, Ralf R. H., Schemmerhofen, GERMANY, FEDERAL
 REPUBLIC OF
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. KG, Ingelheim,
 GERMANY, FEDERAL REPUBLIC OF (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004166125	A1	20040826
APPLICATION INFO.:	US 2003-636088	A1	20030807 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	DE 2002-DE10238470	20020822
	US 2002-409258P	20020909 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	BOEHRINGER INGELHEIM CORPORATION, 900 RIDGEBURY ROAD, P. O. BOX 368, RIDGEFIELD, CT, 06877	
NUMBER OF CLAIMS:	15	
EXEMPLARY CLAIM:	1	
LINE COUNT:	1596	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds of formula (I) ##STR1##

wherein R¹ to R⁴ are defined as in the claims, or the prodrugs or salts thereof, particularly the physiologically acceptable salts thereof, pharmaceutical compositions containing these compounds, and methods of treating type I and type II diabetes mellitus, arthritis, obesity, allograft transplantation, or calcitonin-induced osteoporosis using these compounds.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

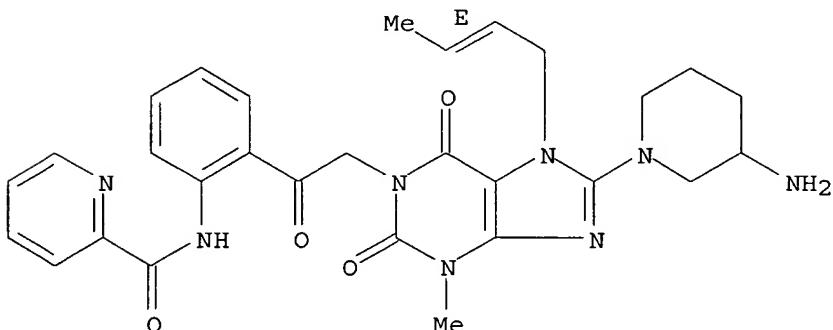
IT 666816-82-6P

(preparation of xanthines as dipeptidylpeptidase IV inhibitors for the treatment of diabetes)

RN 666816-82-6 USPATFULL

CN 2-Pyridinecarboxamide, N-[2-[(8-(3-amino-1-piperidinyl)-7-(2E)-2-butenyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl)acetyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



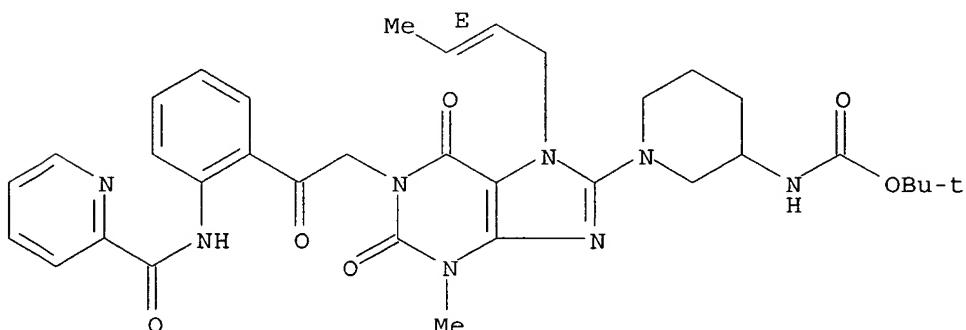
IT 666817-05-6P

(preparation of xanthines as dipeptidylpeptidase IV inhibitors for the treatment of diabetes)

RN 666817-05-6 USPATFULL

CN Carbamic acid, [1-[(7-(2E)-2-butenyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-[2-oxo-2-[(2-pyridinylcarbonyl)amino]phenyl]ethyl]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L36 ANSWER 6 OF 7 USPATFULL on STN

ACCESSION NUMBER: 2004:179045 USPATFULL
 TITLE: Xanthine derivatives, the preparation thereof and their use as pharmaceutical compositions
 INVENTOR(S): Eckhardt, Matthias, Biberach, GERMANY, FEDERAL REPUBLIC OF
 Himmelsbach, Frank, Mittelbiberach, GERMANY, FEDERAL REPUBLIC OF
 Langkopf, Elke, Warthausen, GERMANY, FEDERAL REPUBLIC OF
 Maier, Roland, Biberach, GERMANY, FEDERAL REPUBLIC OF
 Mark, Michael, Biberach, GERMANY, FEDERAL REPUBLIC OF
 Tadayyon, Mohammad, Ulm, GERMANY, FEDERAL REPUBLIC OF
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. KG, Ingelheim,

GERMANY, FEDERAL REPUBLIC OF (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004138215	A1	20040715
APPLICATION INFO.:	US 2003-716141	A1	20031118 (10)
PRIORITY INFORMATION:	DE 2002-10254304	20021121	<i>Hisam</i>
	US 2002-432450P	20021211 (60)	
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		
LEGAL REPRESENTATIVE:	BOEHRINGER INGELHEIM CORPORATION, 900 RIDGEBURY ROAD, P. O. BOX 368, RIDGEFIELD, CT, 06877		
NUMBER OF CLAIMS:	15		
EXEMPLARY CLAIM:	1		
LINE COUNT:	2236		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention relates to substituted xanthines of general formula ##STR1##

the tautomers, the stereoisomers, the mixtures thereof, the prodrugs thereof and the salts thereof, which have valuable pharmacological properties, particularly an inhibitory effect on the activity of the enzyme dipeptidylpeptidase-IV (DPP-IV).

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

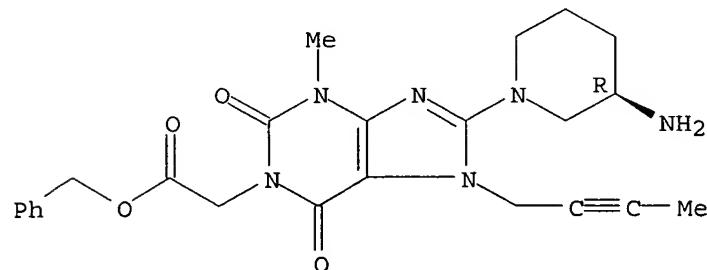
IT 697806-80-7P 697806-84-1P 697806-90-9P
697806-92-1P 697806-93-2P 697806-95-4P
697806-96-5P

(preparation of xanthine derivs. as dipeptidylpeptidase IV inhibitors)

RN 697806-80-7 USPATFULL

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

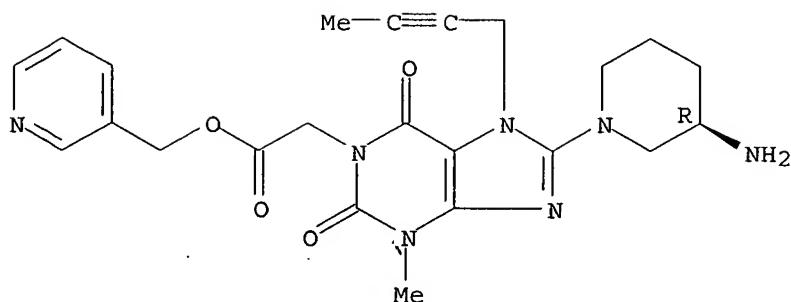
Absolute stereochemistry.



RN 697806-84-1 USPATFULL

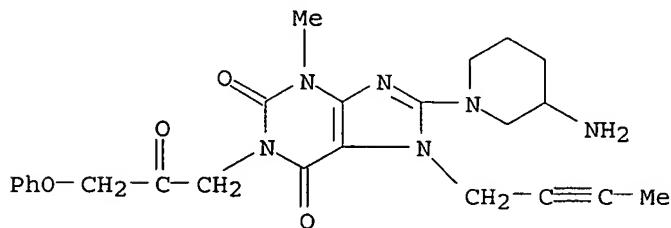
CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, 3-pyridinylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 697806-90-9 USPATFULL

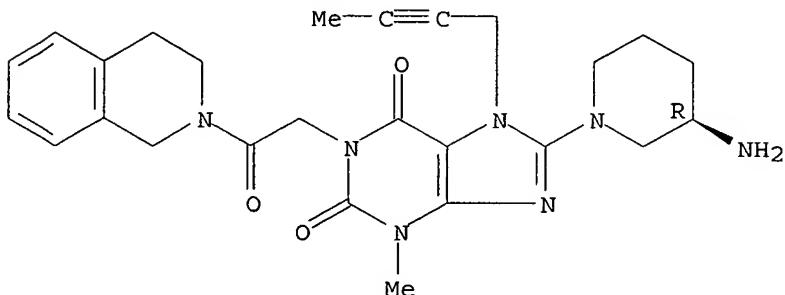
CN 1H-Purine-2,6-dione, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-3,7-dihydro-3-methyl-1-(2-oxo-3-phenoxypropyl)- (9CI) (CA INDEX NAME)



RN 697806-92-1 USPATFULL

CN Isoquinoline, 2-[(8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

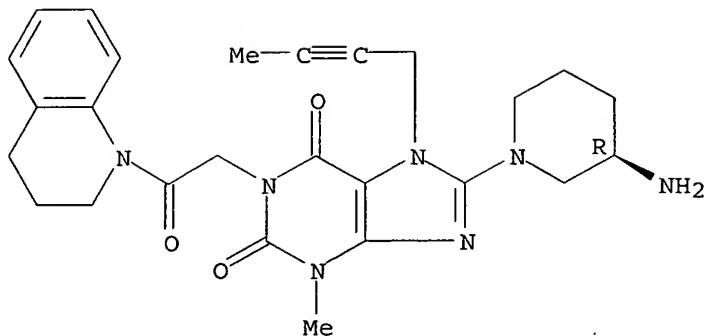
Absolute stereochemistry.



RN 697806-93-2 USPATFULL

CN Quinoline, 1-[(8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

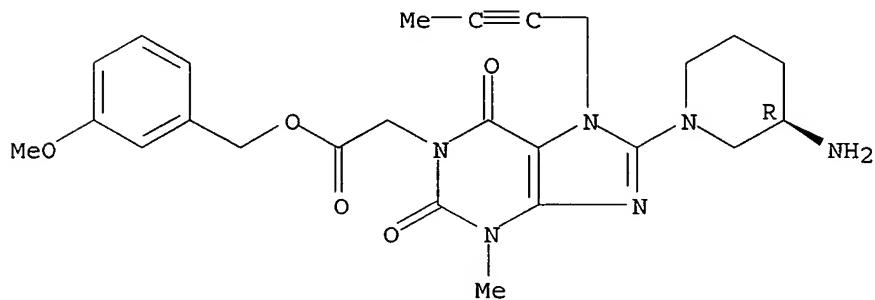
Absolute stereochemistry.



RN 697806-95-4 USPATFULL

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

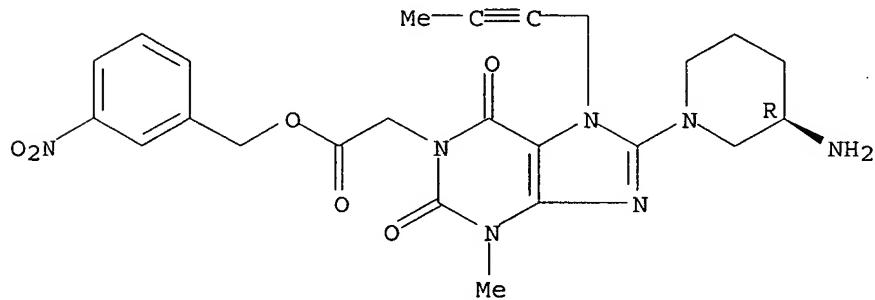
Absolute stereochemistry.



RN 697806-96-5 USPATFULL

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

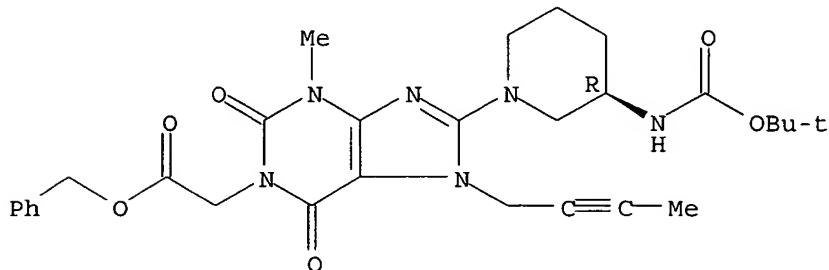
IT 697806-55-6P 697806-59-0P 697806-67-0P
697806-68-1P 697806-72-7P 697806-75-0P
697806-76-1P

(preparation of xanthine derivs. as dipeptidylpeptidase IV inhibitors)

RN 697806-55-6 USPATFULL

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

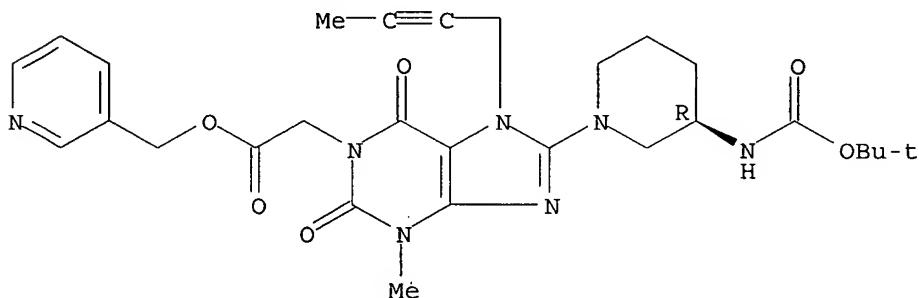
Absolute stereochemistry.



RN 697806-59-0 USPATFULL

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, 3-pyridinylmethyl ester (9CI) (CA INDEX NAME)

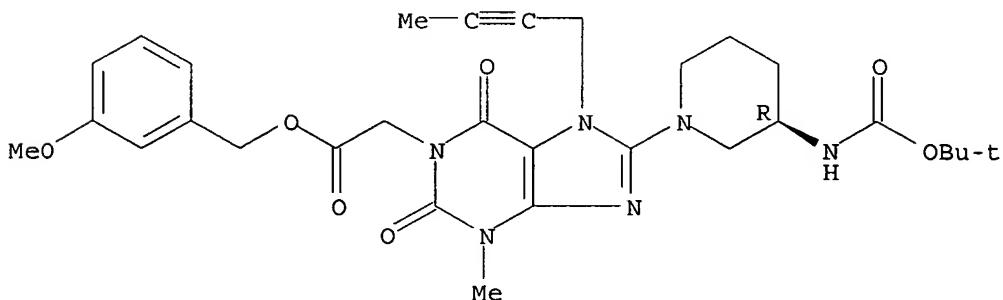
Absolute stereochemistry.



RN 697806-67-0 USPATFULL

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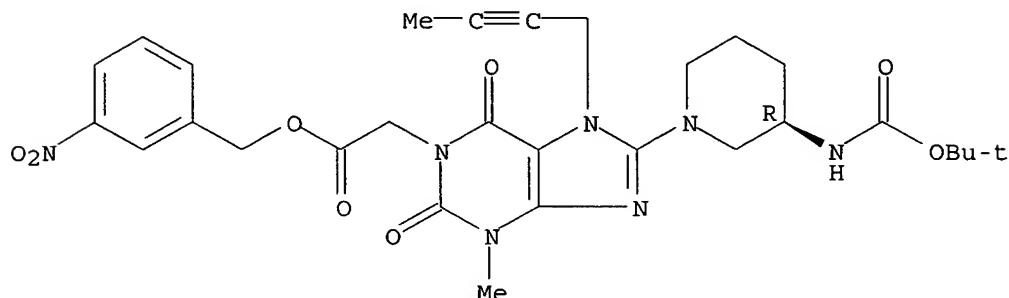
Absolute stereochemistry.



RN 697806-68-1 USPATFULL

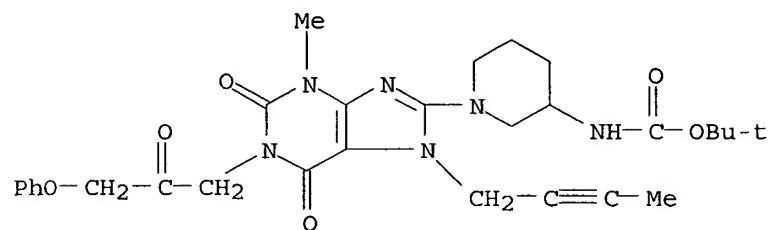
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Absolute stereochemistry.



RN 697806-72-7 USPATFULL

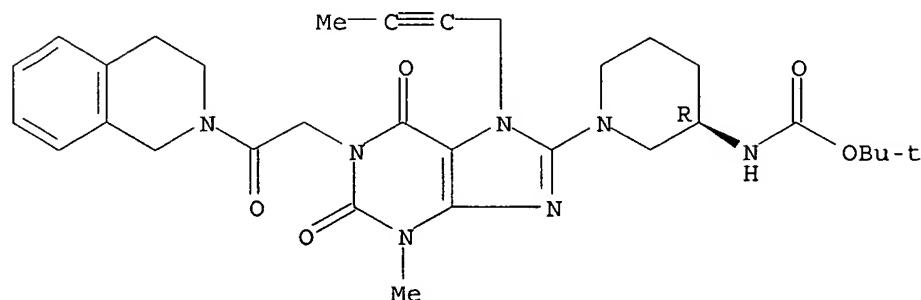
CN Carbamic acid, [1-[7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-3-phenoxypropyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 697806-75-0 USPATFULL

CN Carbamic acid, [(3R)-1-[7-(2-butynyl)-1-[2-(3,4-dihydro-2(1H)-isoquinolinyl)-2-oxoethyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

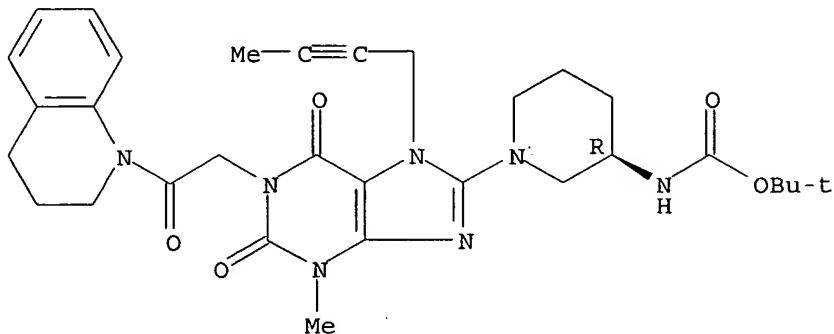


RN 697806-76-1 USPATFULL

CN Carbamic acid, [(3R)-1-[7-(2-butynyl)-1-[2-(3,4-dihydro-1(2H)-quinolinyl)-2-oxoethyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl]-3-

piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L36 ANSWER 7 OF 7 USPATFULL on STN

ACCESSION NUMBER: 2004:108168 USPATFULL

TITLE: Xanthine derivative and DPPIV inhibitor

INVENTOR(S): Yoshikawa, Seiji, Ibaraki, JAPAN

Emori, Eita, Ibaraki, JAPAN

Matsuura, Fumiyo, Ibaraki, JAPAN

Clark, Richard, Ibaraki, JAPAN

Ikuta, Hironori, Ibaraki, JAPAN

Yasuda, Nobuyuki, Ibaraki, JAPAN

Nagakura, Tadashi, Ibaraki, JAPAN

Yamazaki, Kazuto, Ibaraki, JAPAN

Aoki, Mika, Ibaraki, JAPAN

PATENT ASSIGNEE(S): Eisai Co., Ltd., Tokyo, JAPAN, 112-8088 (non-U.S. corporation)

NUMBER KIND DATE

PATENT INFORMATION: US 2004082570 A1 20040429

APPLICATION INFO.: US 2003-374918 A1 20030224 (10)

NUMBER DATE

PRIORITY INFORMATION: JP 2002-47761 20020225

JP 2002-149557 20020523

DOCUMENT TYPE: Utility

FILE SEGMENT: APPLICATION

LEGAL REPRESENTATIVE: TOWNSEND AND TOWNSEND AND CREW, LLP, TWO EMBARCADERO CENTER, EIGHTH FLOOR, SAN FRANCISCO, CA, 94111-3834

NUMBER OF CLAIMS: 27

EXEMPLARY CLAIM: 1

LINE COUNT: 7402

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides novel compounds exhibiting an excellent DPPIV inhibition effect.

The compounds are represented by the formula: ##STR1##

wherein, m is 0 or 1;

n is 0;

R.³¹, R.³², R.³³, R.³⁴, R.³⁵, R.³⁶, R.³⁷, R.³⁸, R.³⁹, R.⁴⁰, R.⁴¹, and R.⁴² each represent a hydrogen atom;

X represents an alkynyl group, an aryl group, and such, which group may be substituted; and,

R.¹ and R.² each independently represents a hydrogen atom, an alkyl group, an alkoxy group, or such,

or salts or hydrates thereof.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 586402-89-3P

(preparation of xanthine derivs. as DPPIV inhibitors)

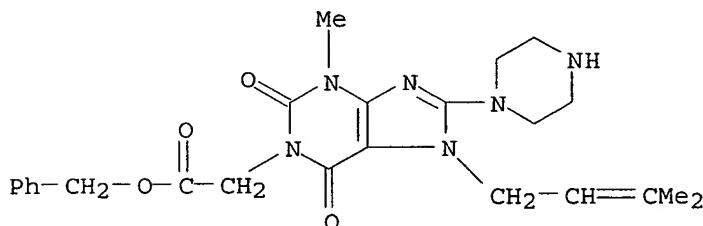
RN 586402-89-3 USPATFULL

CN 1H-Purine-1-acetic acid, 2,3,6,7-tetrahydro-3-methyl-7-(3-methyl-2-butenyl)-2,6-dioxo-8-(1-piperazinyl)-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 586402-88-2

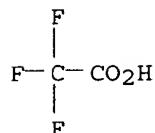
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CM 2

CRN 76-05-1

CMF C2 H F3 O2



Structure search in BEILSTEIN

Berch 10_716141

12/15/2005

> file beilstein

FILE 'BEILSTEIN' ENTERED AT 16:46:16 ON 15 DEC 2005

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FILE LAST UPDATED ON OCTOBER 10, 2005

FILE COVERS 1771 TO 2005.

*** FILE CONTAINS 9,363,954 SUBSTANCES ***

>>> PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE, THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *

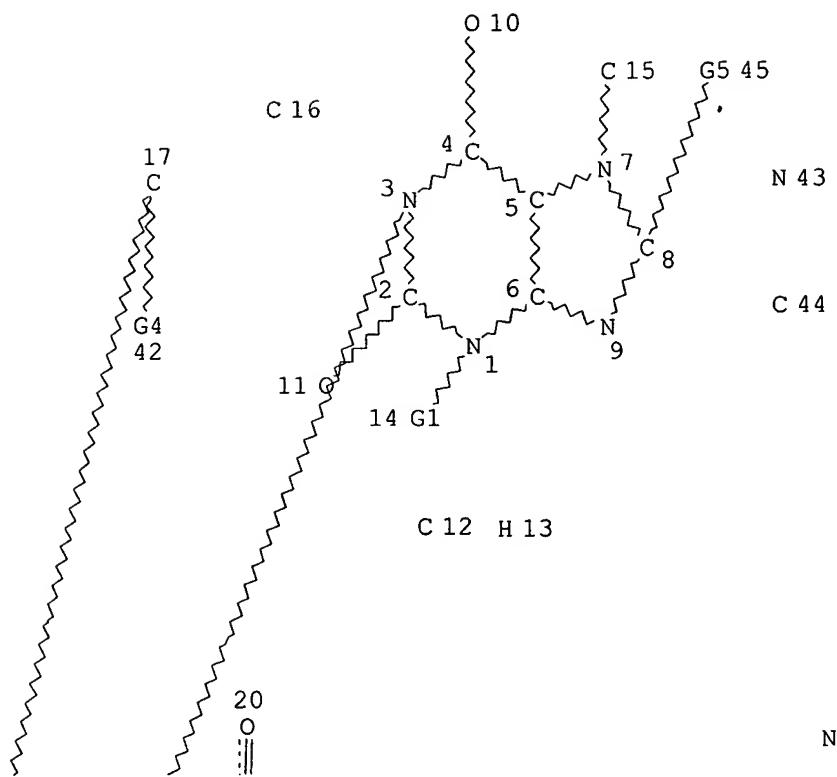
NEW

* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE
SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,
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Berch 10_716141

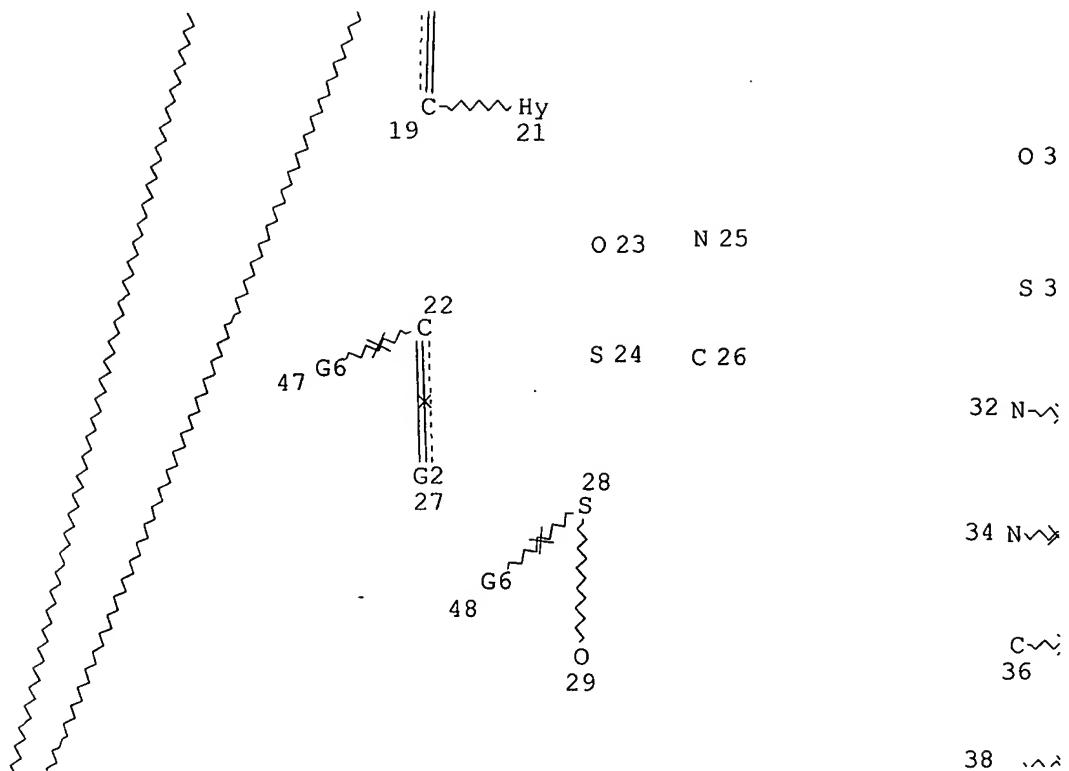
12/15/2005



Page 1-A

6

Page 1-B



Page 2-A
30

31

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~> .

Page 2-B

18 G20

38 C~;

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Page 3-A

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~~N 41

Page 3-B
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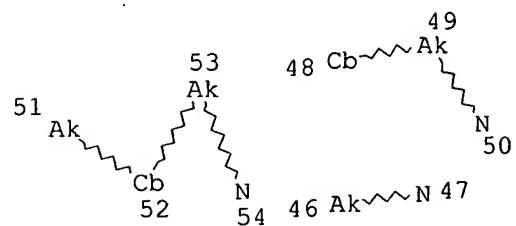
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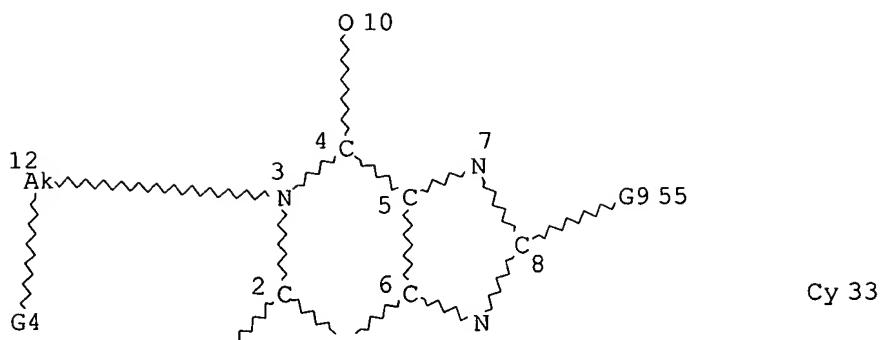
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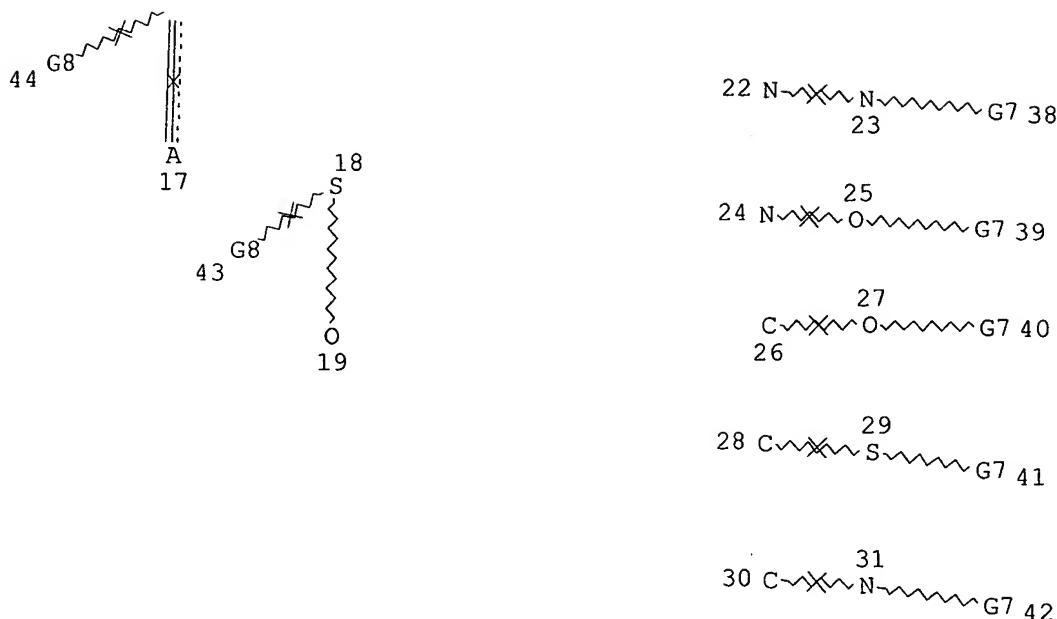
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35 Ak ~~~~~ Cy 34



Page 2-A



Page 3-A

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0 ANSWERS

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12/15/2005

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FILE 'CAPLUS' ENTERED AT 11:24:48 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 11:24:49 ON 15 DEC 2005

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FILE 'REGISTRY' ENTERED AT 16:20:45 ON 15 DEC 2005
FILE 'STNGUIDE' ENTERED AT 16:20:48 ON 15 DEC 2005
FILE 'REGISTRY' ENTERED AT 16:24:10 ON 15 DEC 2005
L27 STRUCTURE uploaded
L28 3 SEA SUB=L14 SSS SAM L27
D SCA
L29 29 SEA SUB=L14 SSS FUL L27
D SCA
SAVE TEMP L29 BER141STRH/A
FILE 'CAPLUS' ENTERED AT 16:33:46 ON 15 DEC 2005
L30 4 SEA ABB=ON PLU=ON L29

FILE 'BEILSTEIN' ENTERED AT 16:35:09 ON 15 DEC 2005
L31 0 SEA SSS FUL L27
L32 3 SEA SSS FUL L12
L33 0 SEA SUB=L32 SSS FUL L27

FILE 'MARPAT' ENTERED AT 16:37:11 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 16:37:43 ON 15 DEC 2005
L34 ANALYZE PLU=ON L29 1- LC : 3 TERMS
D

FILE 'USPATFULL' ENTERED AT 16:38:04 ON 15 DEC 2005
L35 3 SEA ABB=ON PLU=ON L29

FILE 'STNGUIDE' ENTERED AT 16:40:42 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 16:41:05 ON 15 DEC 2005
D STAT QUE L29
D L34

FILE 'CAPLUS' ENTERED AT 16:42:31 ON 15 DEC 2005
D QUE NOS L30
D QUE NOS L35

FILE 'REGISTRY' ENTERED AT 16:43:20 ON 15 DEC 2005
D STAT QUE L29
D L34

FILE 'CAPLUS' ENTERED AT 16:43:38 ON 15 DEC 2005
D QUE NOS L30

FILE 'USPATFULL' ENTERED AT 16:43:50 ON 15 DEC 2005
D QUE NOS L35

FILE 'CAPLUS, USPATFULL' ENTERED AT 16:44:10 ON 15 DEC 2005
L36 7 DUP REM L30 L35 (0 DUPLICATES REMOVED)
ANSWERS '1-4' FROM FILE CAPLUS
ANSWERS '5-7' FROM FILE USPATFULL
D IBIB ABS HITSTR L36 1-7

FILE 'STNGUIDE' ENTERED AT 16:46:02 ON 15 DEC 2005

FILE 'BEILSTEIN' ENTERED AT 16:46:16 ON 15 DEC 2005
D STAT QUE L33

FILE 'STNGUIDE' ENTERED AT 16:49:49 ON 15 DEC 2005

FILE HOME

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Dec 9, 2005 (20051209/UP).

FILE CAPLUS

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FILE COVERS 1907 - 15 Dec 2005 VOL 143 ISS 25
FILE LAST UPDATED: 14 Dec 2005 (20051214/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 DEC 2005 HIGHEST RN 869939-98-0
DICTIONARY FILE UPDATES: 14 DEC 2005 HIGHEST RN 869939-98-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE LREGISTRY

LREGISTRY IS A STATIC LEARNING FILE

NEW CAS INFORMATION USE POLICIES, ENTER HELP USAGETERMS FOR DETAILS.

FILE BEILSTEIN

FILE LAST UPDATED ON OCTOBER 10, 2005

FILE COVERS 1771 TO 2005.

FILE CONTAINS 9,363,954 SUBSTANCES

>>> PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

 * PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
 * SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE . *
 * ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
 * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
 * FOR PRICE INFORMATION SEE HELP COST *

NEW
 * PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE
 SEARCHED, SELECTED AND TRANSFERRED.
 * NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,
 ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A
 COMPOUND AT A GLANCE.

FILE MARPAT
 FILE CONTENT: 1988-PRESENT (VOL 143 ISS 24) (20051211/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
 (COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6943267 13 SEP 2005
 DE 1020040544 15 SEP 2005
 EP 1577935 21 SEP 2005
 JP 2005272454 06 OCT 2005
 WO 2005097137 20 OCT 2005

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

MARPATpreviews will be removed from STN on December 31, 2005.

FILE USPATFULL
 FILE COVERS 1971 TO PATENT PUBLICATION DATE: 15 Dec 2005 (20051215/PD)
 FILE LAST UPDATED: 15 Dec 2005 (20051215/ED)
 HIGHEST GRANTED PATENT NUMBER: US6976271
 HIGHEST APPLICATION PUBLICATION NUMBER: US2005278816
 CA INDEXING IS CURRENT THROUGH 15 Dec 2005 (20051215/UPCA)
 ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 15 Dec 2005 (20051215/PD)
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2005
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2005

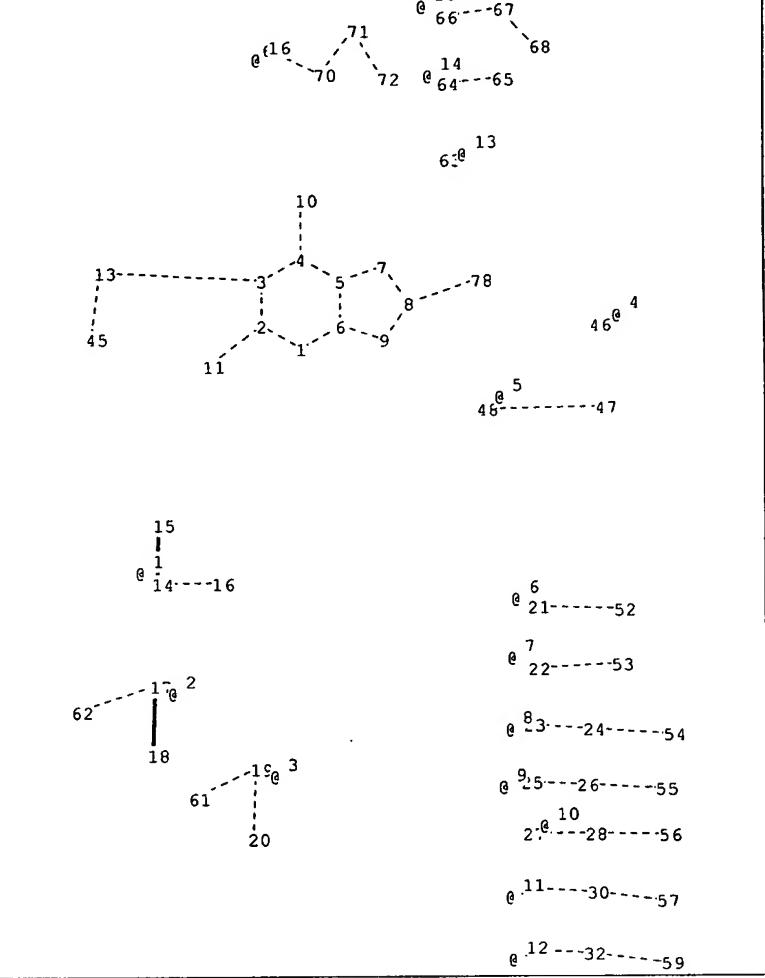
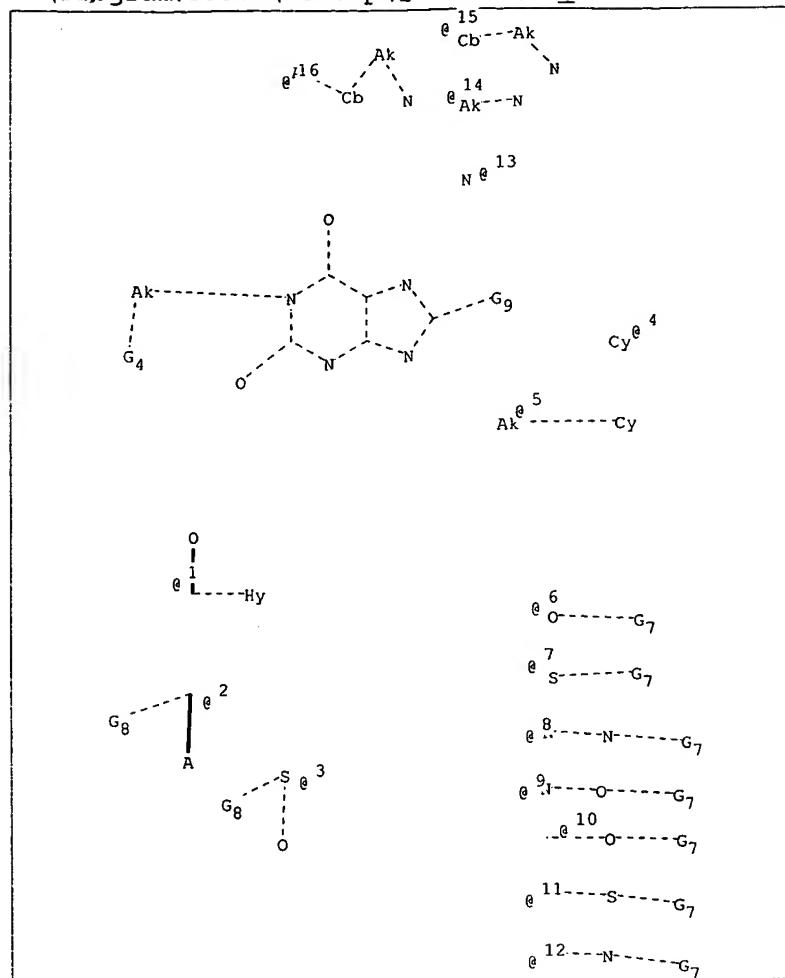
>>> USPAT2 is now available. USPATFULL contains full text of the <<<
 >>> original, i.e., the earliest published granted patents or <<<

>>> applications. USPAT2 contains full text of the latest US <<<
>>> publications, starting in 2001, for the inventions covered in <<<
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
>>> enter this cluster. <<<
>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=



chain nodes :

10 11 13 14 15 16 20 45 46 47 48 52 53 54 55 56 57 59 64 66 67 69
70 71 78

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

17 18 19 21 22 23 24 25 26 27 28 29 30 31 32 61 62 63 65 68 72

chain bonds :

2-11 3-13 4-10 8-78 13-45 14-15 14-16 19-20 21-52 22-53 24-54 26-55 28-56
 30-57 32-59 47-48 64-65 66-67 67-68 69-70 70-71 71-72

ring/chain bonds :

17-18 17-62 19-61 23-24 25-26 27-28 29-30 31-32

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-2	1-6	2-3	2-11	3-4	3-13	4-5	4-10	5-6	5-7	6-9	7-8	8-9	8-78	13-45	14-15
14-16	17-18	17-62	19-20	19-61	21-52	22-53	23-24	24-54	25-26	26-55	27-28	28-56			
29-30	30-57	31-32	32-59	47-48	64-65	66-67	67-68	69-70	70-71	71-72					

G4 : [*1], [*2], [*3]

G7 : [*4], [*5]

G8 : [*6], [*7], [*8], [*9], [*10], [*11], [*12]

G9: [*13], [*14], [*15], [*16]

Connectivity :

2:3 E exact RC ring/chain 4:3 E exact RC ring/chain 9:2 E exact RC ring/chain
10:1 E exact RC ring/chain 11:1 E exact RC ring/chain 20:1 E exact RC ring/chain

Match level :

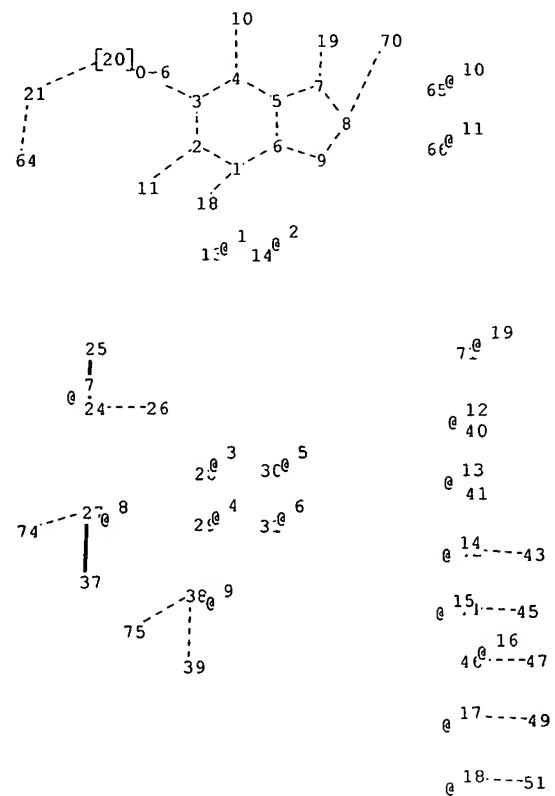
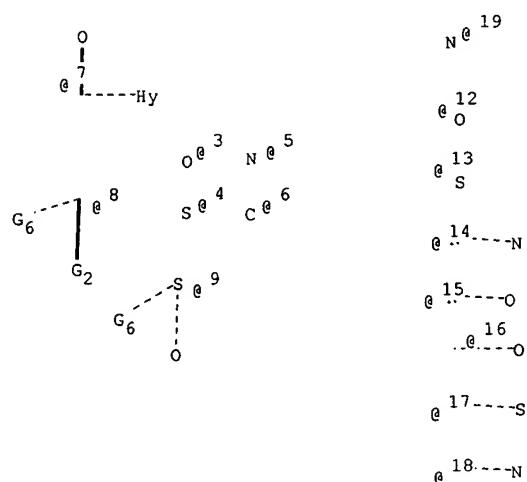
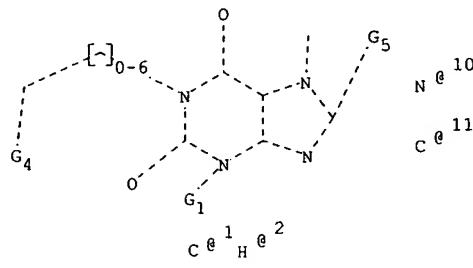
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 52:CLASS 53:CLASS
54:CLASS 55:CLASS 56:CLASS 57:CLASS 59:CLASS 61:CLASS 62:CLASS 63:CLASS 64:CLASS
65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:Atom 71:CLASS 72:CLASS 78:CLASS

Generic attributes :

16:
Saturation : Unsaturated
Number of Hetero Atoms : less than 2
Type of Ring System : Polycyclic
46:
Saturation : Unsaturated
47:
Saturation : Unsaturated

Element Count :

Node 16: Limited
N, N1



chain nodes :

10 11 14 18 20 21 24 25 26 39 64 70

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

13 19 27 28 29 30 31 37 38 40 41 42 43 44 45 46 47 48 49 50 51 65
66 71 74 75

chain bonds :

1-18 2-11 3-20 4-10 7-19 8-70 20-21 21-64 24-25 24-26 38-39

ring/chain bonds :

27-37 27-74 38-75 42-43 44-45 46-47 48-49 50-51

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-2 1-6 1-18 2-3 2-11 3-4 3-20 4-5 4-10 5-6 5-7 6-9 7-8 7-19 8-9 8-70
20-21 21-64 24-25 24-26 27-37 27-74 38-39 38-75 42-43 44-45 46-47 48-49 50-51

G1: [*1], [*2]

G2: [*3], [*4], [*5], [*6]

G4: [*7], [*8], [*9]

G5: [*10], [*11]

G6: [*12], [*13], [*14], [*15], [*16], [*17], [*18], [*19]

Connectivity :

2:3 E exact RC ring/chain 4:3 E exact RC ring/chain 9:2 E exact RC ring/chain
10:1 E exact RC ring/chain 11:1 E exact RC ring/chain 39:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 13:CLASS 14:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 24:CLASS 25:CLASS
26:Atom 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 37:CLASS 38:CLASS 39:CLASS
40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS
49:CLASS 50:CLASS 51:CLASS 64:CLASS 65:CLASS 66:CLASS 70:CLASS 71:CLASS 74:CLASS
75:CLASS

Generic attributes :

26:
Saturation : Unsaturated
Number of Hetero Atoms : less than 2
Type of Ring System : Polycyclic

Element Count :

Node 26: Limited
N,N1